Final Report for Period: 07/2007 - 06/2008

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Principal Investigator: Ye, Wenjing .

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Organization: GA Tech Res Corp - GIT

Submitted By:

White, Jacob - Co-Principal Investigator

Title:

Numerical Techniques for Extracting System-Level Models of Micromachined Devices

Project Participants

Senior Personnel

Name: Ye, Wenjing

Worked for more than 160 Hours: Yes

Contribution to Project:

Name: White, Jacob

Worked for more than 160 Hours: Yes

Contribution to Project:

Post-doc

Graduate Student

Name: Ding, Jian

Worked for more than 160 Hours: Yes

Contribution to Project:

Ms. Jian Ding is responsible for the implementation of the BEM solver for nonlinear problems. She has been supported as GRA through this grant since July 2003.

Name: Vasilyev, Dmitry

Worked for more than 160 Hours: Yes

Contribution to Project:

Dmitry Vasilyev is working on the general model reduction problem. He is partially supported by this project.

Name: Coelho, Carlos

Worked for more than 160 Hours: Yes

Contribution to Project:

Carlos Coelho is working on interal equation technique for fluids with extensions to mixing.

Name: Masters, Nathan

Worked for more than 160 Hours: No

Contribution to Project:

Nathan is working on molecular simulation of gas flows and hybrid BEM/DSMC methods. He is partially supported by this grant.

Name: Lee, Jung Hoon

Worked for more than 160 Hours: No

Contribution to Project:

Jung Hoon is working on the combination of optimization and model reduction.

Undergraduate Student

Name: Cavin, Kyle

Worked for more than 160 Hours: No

Contribution to Project:
Kyle is working on molecular simulation of gas flows and hybrid BEM/DSMC methods. He is the REU participant.

Technician, Programmer

Other Participant

Research Experience for Undergraduates

Organizational Partners

Inst. of Mech., Chinese Academy of Sci.
Please see the 'activities' section.

Other Collaborators or Contacts

Professors Denny Freeman and Salil Dasai at MIT: involved in experimental validation.

Dr. Leonard Gray at Oak Ridge National Laboratory: involved in nonlinear BEM.

Activities and Findings

Research and Education Activities:

The objectives of this three-year project are to develop fast integral equation based solvers for non-linear problems, led by Georgia Tech group, and to interface these fast nonlinear solvers with model reduction techniques, led by MIT group. The goal is to automatically extract macro models suitable for system-level modeling and optimization. The target applications are problems with 3-D complicated geometries such as those encountered in Microsystems.

The activities in the first year (2003-2004) focused on (1) developing efficient volume integration techniques based on the precorrected-FFT acceleration technique and (2) methods for generating reduced models for a class of nonlinear dynamical systems, based on truncated balanced realization (TBR) algorithm and a recently developed trajectory piecewise-linear (TPWL) model order reduction approach.

Activities in the second year (2004-2005) have focused on developing (1) efficient solvers for 3-D nonhomogeneous and nonlinear problems based on integral equations and the volume integration techniques developed in the first year and (2) new approaches of model order reduction and improved Fast Stokes solvers based on modified Green's function. The education and outreach activities in this year focus on student training and research experience for graduate and undergraduate students through international collaboration.

Activities in last years were concentrated on developing efficient molecular based simulation methods (Octant Flux Splitting Information Preserving Direct Simulation Monte Carlo) for submicron gas transport and the applications of these methods to the modeling of various MEMS devices.

Findings:

Fast Integral Based Solvers

In order to develop an integral based solver for nonhomogeneous and/or nonlinear problems, an integral representation of the underlying governing equation, often in a differential form, must be first developed. While such an integral representation is relatively easy to formulate for linear problems, it is in general difficult for nonlinear problems because of the lack of the Greens' functions or the fundamental solutions. The approach we employed is to formulate the integral representation based on the Greens' function of the corresponding linear operator and casting the nonlinear (or nonhomogeneous) term as the body force. Such an approach is applicable to any nonlinear problems as long as there is a linear operator in the equation and the corresponding Greens function exists. The resulting integral formulation contains a volume integral and this integral is evaluated using the 'grid-based' approach that we developed in the first year of this project. To investigate the effect of the approximation errors introduced in the evaluation of volume integrals on the overall accuracy of the solver, 3-D Poisson problems were chosen as the first testing vehicle. Domains ranging from a simple sphere to a multiply-connected domain (please refer to the attached Fig. 1) were tested. Satisfactory accuracy and efficiency have been achieved. In particular, when compared to several competing integral based methods such as the Dual Reciprocity method (a meshless method) and the Auxiliary Domain Subtraction Method, our approach performs the best in terms of the ratio of error to the overall CPU time. Detailed description of this work is given in publication [3]. With the confidence gained from the performance of the developed Poisson solvers, we then moved onto Helmholtz problems and quasilinear Laplace problems. For these problems, the integrand in the volume integrals which contains the nonhomogeheous term or the nonlinear termdepends on the unknown function. A successive relaxation scheme was employed to iteratively solve the corresponding integral equation. On all cases that have been tested including the one with a multiply-connected domain, the total number of iterations to achieve a convergence with a relative tolerance of 0.001 is less than 6, indicating the approximation error in the volume integration does not affect the convergence of the relaxation scheme when applied to our testing problems, particularly the quasilinear Laplace problems. The performances of the developed solvers in both Helmholtz and quasilinear Laplace problems are comparable to that of Poisson problems. Preliminary results were presented in publications [4]. A journal paper has been submitted on this subject. showing the performance comparison of our solver, denoted as 'GIM', with the competing method, denoted as 'ADM', for the Helmholtz problem in a multiply-connected domain. As indicated in the plot, our approach requires much less CPU time for a given error.

Model Order Reduction

On reduced models, a method based on truncated balanced realization (TBR) algorithm and a trajectory piecewise-linear (TPWL) model order reduction approach has been developed. A comparison between schemes using both Krylov-based and TBR-based projections was also conducted. Computational results, obtained for examples of nonlinear circuits and a micro-electro-mechanical system (MEMS), indicate that the TBR reduction scheme generates nonlinear macromodels with superior accuracy as compared to reduction algorithms based solely on Krylov subspace projections, while maintaining a relatively low model extraction cost.
Model order reduction is a key technique for generating efficient models micromachined devices, but the existing methods have difficulties with problems which are innately nonsymmetric, like high frequency interconnect or coupled-domain micromachined device problems. The difficulty is that the most widely used techniques, be they based on Krylov subspaces or collections of frequency domain solutions, effectively seperately obtain the most controllable and most observable subspaces. What is needed for model order reduction is the dominant subspace of the product of controllability and observability. We are investigating a fast method for directly computing the dominant subspace of the product using what is effectively a power method with approximations. Preliminary results suggest that the method can be far more effective than existing techniques on

nonsymmetric examples.

Fluid Analysis

Fluid flow in micromachined devices is almost always bounded below by a substrate, and many fluidic microdevices function by using wide structures which form a small fluid gap with the substrate. Our fast fluids analysis program, FastStokes, must use discretization panels that are commensurate with the gap size, and therefore an enormous number of panels are needed to discretize any realistic structure. We have been developing an approach based on building the substrate into the Stokes flow Green's function in order to eliminate this problem. Preliminary results demonstrate that our approach also eliminates a troublesome null space in the Stokes' flow operator.

Efficient Molecular Based Simulation Methods for Submicron Gas Transport and their Applications in Micro Devices

When the minimum feature size of micromachined devices is smaller than 1 μm and/or when these devices are operated in a low pressure environment, the rarefaction effect of gas becomes important and the classical Navier-Stokes equations are no longer accurate for the prediction of gas transport. Modifications to Navier-Stokes equations must be made in order to capture non-continuum effects. However, this has proven to be quite challenging particularly when rarefaction is significant. Despite a lot of efforts that have been made, a close set of continuum equations that is capable of describing gas flows at any regime is yet to come. Another and perhaps more natural type of approaches are molecular based approaches. The direct simulation Monte Carlo (DSMC) is regarded as the most general method for the modeling of rarefied gas. It is similar to the molecular dynamics (MD) method, but much more efficient. Instead of tracking the motion of each real molecule as it is in the MD method, the DSMC tracks the motion of each simulation molecule which is a statistical representation of a large cluster of real molecules. Because of that, it is possible to simulate relatively large system using the DSMC. However, a major challenge that the DSMC faces when employed to simulate micro/nano gas flows is the statistical noise, which is often several orders larger than the macroscopic quantities of interest, for example, the separation rate. The standard approach for the reduction of noise is to perform time averaging for steady problems and ensemble averaging for unsteady problems. For low-speed micro/nano gas flows, the required sample size is often on the order of , making the DSMC impractical for the modeling and design of MEMS devices. We have developed an efficient DSMC method, the octant flux splitting information preserving DSMC (OSIP-DSMC), to overcome the low-efficiency issue. Compared with various other methods either DSMC based or non-DSMC based, our method is the only one that can model highly rarefied and highly non-equilibrium (large thermal gradient) gas flows in a general setting. Figure 1 shows the velocity field of air inside a micro channel with one hot end (T = 573 K) and one cold end (T = 273 K). Due to thermal transpiration, air will flow from the cold end to the hot end near the channel walls and move from the hot end to the cold end at the center of the channel due to the accumulated pressure gradient. While the DSMC results showed noticeable noise, the OFIP-DSMC results clearly showed the expected circulation flow. The method was then applied to model a Knudsen pump fabricated by Prof. GianchandaniÆs group (University of Michigan). The measured pressure difference is 0.46 atm while the OSIP-DSMC modeling predicts a 0.31 atm pressure difference. The discrepancy between the two results is likely caused by the error in the temperature profile of the channel which was obtained indirectly from a solid-phase heat transfer model of the device. The OSIP-DSMC was also applied to model gas-phase heat transfer inside a thermal sensing Atomic Force Microscope. Circulation flows around the end of the cantilever were observed at the stead state. Those flows are caused by a combination of thermal transpiration and thermal stress. Another interesting finding is the non-zero net pressure acting on the cantilever obtained from the simulation. This non-zero net pressure exerts a force on the cantilever and causes the cantilever to deform. Such a force is called Knudsen force and has been experimentally observed and measured.

Training and Development:

Six Ph.D. students were partially supported through this grant. They were actively involved in the research activities described in the previous section. Among them, one is a female student (Mrs. Jian Ding) who has recently been granted the doctoral degree from Georgia Institute of Technology.

Outreach Activities:

With the supplementary award, a trip to Institute of Mechanics, Chinese Academy of Science was taken in place during September 2004. A graduate student, Nathan Masters, and an undergraduate student, Kyle Cavin, together with Prof. Ye visited Drs. Fan Jing and Ching Shen's groups. During the two-week stay, our students worked and socialized closely with researchers and their students at Institute of Mechanics. Several seminars were given by students on both sides and daily group meeting was held. The scientific objective of this collaboration is to develop hybrid continuum-molecular approaches for multiscale problems in MEMS/NEMS systems by interfacing integral approaches developed in this project with the Direct Simulation of Monte Carlo (DSMC), a molecular approach. Our students have learned a great deal of DSMC method from the experts Drs. Fan Jing and Chin Shen. Nathan and Kyle developed a graphic interface for molecular simulation of rarefied gas using the DSMC method. This interactive interface allows the potential users to enter input parameters, to select boundary conditions and output modes on a single window. It is a part of our simulation package that will be made available to the public (subject to the regulation of Georgia Institute of Technology). The visit was fruitful scientifically as well as culturally. Our students had a chance to visit several historic sites in Beijing, for example, the famous Great Wall, the Forbidden City, etc. As pointed our by Kyle, the trip to Beijing was nothing short of an odyssey. Truly, this trip has provided them a very different perspective about the world.

Journal Publications

N. Masters and W. Ye, "Fast BEM Solution for Coupled 3D Electrostatic and Linear Elastic Problems", Engineering Analysis with Boundary Elements, p. 1175, vol. 28, (2004). Published,

N. Masters, W. Ye and W. King, "Heat Transfer in Thermal Sensing Atomic Force Microscopy: Non-Continuum Effects and Sensitivity Analysis", Technical Proceedings of the Transport Phenomena in Micro and Nanodevices, p. 10, vol. III, (2004). Published,

J. Ding, W. Ye and L. Gray, "An Accelerated Surface Discretization Based BEM Approach for Non-homogenous Linear Problems in 3-D Complex Domain", International Journal for Numerical Methods in Engineering, p. 1775, vol. 63, (2005). Published,

J. Ding and W. Ye, "Boundary Integral Solution of Quasi-linear Laplace Equation", Proc. of Modeling and Simulation of Microsystems, p. , vol. , (2005). Accepted,

J. White, "CAD Challenges in BioMEMS Design", Proceedings of the Design Automation Conference, p. 629, vol. , (2004). Published,

C. Coelho, S. Desai, D. Freeman, and J. White, "A Robust Approach for Estimating Diffusion Constants from Concentration Data in Microchannel Mixers", Proc. of Modeling and Simulation of Microsystems, p. , vol. , (2005). Accepted,

J. H. Lee, D. Vasilyev, A. Vithayathil, L. Daniel, and J. White, "Accelerated Optical Topography Inspection Using Parameterized Model Order Reduction", Proceedings of the IEEE International Microwave Symposium, p. , vol. , (2005). Accepted,

N. Masters, W. Ye and W. King, "The Impact of Sub-continuum Gas Conduction on Topography Measurement Sensitivity Using Heated Atomic Force Microscope Cantilevers", Physics of Fluids, p. 100615, vol. 17, (2005). Published,

J. Ding and W. Ye, "A Grid Based Integral Approach for Quasilinear Problems", Computational Mechanics, p. 113, vol. 38, (2006). Published,

X. Wang, J. White, J. Kanapka, W. Ye and N. Aluru, "Algorithms in FastStokes and its Applications to Micromachined Device Simulation", IEEE Transactions on Computer Aided Design of Integrated Circuits and Systems, p. 248, vol. 25, (2006). Published,

N. Masters and W. Ye, "Octant Flux Splitting Information Preservation DSMC Method for Thermally Driven Flows", Journal of Computational Physics, p. 457, vol. 42, (2007). Published,

D. Vasilyev, M. Rewienski, J. White, "A TBR-based based Trajectory Piecewise-Linear Algorithm for Generating Accurate Low-order Models for Nonlinear Analog Circuits and MEMS", Proceedings of the Design Automation Conference, p. 438, vol. , (2003). Published,

J. Ding and W. Ye, "A Novel Approach for Volume-Integral Evaluation in the BEM", Proceedings of Modeling and Simulation of Microsystems, Boston, p. , vol. , (2004). Published,

C. P. Coelho, J. K. White and L. M. Silveira, "Dealing with Stiffness in Time - Domain Stokes Flow Simulation",", Proceedings of Modeling and Simulation of Microsystems, Boston, p. , vol. , (2004). Published,

Books or Other One-time Publications

X. Wang, J. White, J. Kanapka, W. Ye and N. Aluru, "Algorithms in FastStokes and its Applications to Micromachined Device Simulation", (2006). Book, Published
Editor(s): K. Chakrabarty and J. Zeng
Collection: Design Automation Methods and Tools for Microfluidics-Based Biochips
Bibliography: xxx

W. Ye, "The Boundary Element Method and its Applications to the Modeling of MEMS Devices", (2008). Book, Accepted
Editor(s): Dongqing Li
Collection: Encyclopedia of Micro-Fluidics and Nano-Fluidics
Bibliography: xxxx

Web/Internet Site

Other Specific Products

Product Type:

Software (or netware)

Product Description:

"FastPoisson" A 3-D Integral-Approach based Solver for Poisson Problems

Sharing Information:

The solver is free to teh public subject to regulation of Georgia Institute of Technology.

Product Type:

Software (or netware)

Product Description:

"FastQuasilinear" A 3-D Integral Approach based Solver for Generalized Quasilinear Problems.

Sharing Information:

The solver is free to teh public subject to regulation of Georgia Institute of Technology.

Product Type:

Software (or netware)

Product Description:

"FastStokes" A 3-D Solver for Stokes Problems

Sharing Information:

It is free to the public subject to regulation of MIT.

Contributions

Contributions within Discipline:

Accelerated integral-based approaches have the advantages in their simplicity in mesh generation and their efficiency in system solver due to the built-in acceleration schemes. These two attributes make integral methods particularly attractive for large-scale problems with 3-D complex geometry. Successful applications of these methods have been demonstrated in a variety of engineering problems. However, most of them are linear and homogeneous problems. We have, for the first time, extended accelerated integral approaches to nonhomogeneous/nonlinear problems and have obtained promising results on a set of testing problems. Such a contribution would lead to a much broad scope of applications such as transport analysis of fluid in microfluidic systems, nonlinear fracture analysis, design of functional graded materials for space applications, etc. As we have been working to develop predictive models for bioMEMS devices, we have been collaborating with Professor Freeman and Salil Desai to connect simulation with measurements. Due to this interaction, we have been examining some numerical issues associated with processing the measurements, and generated two new techniques. We developed a robust and geometry independent method for the estimation of diffusion coefficients of solutes from image data. Our diffusion coefficient estimation algorithm works in two steps. First, given the device geometry and the pressure boundary conditions, we calculate the fluid velocity in the device by solving a Stokes flow problem. Then, using the calculated fluid velocity and the concentration at the device inlet and outlet ports, we calculate the solute concentration in the device by solving the convection diffusion problem with a finite differences solver. The diffusion coefficient is estimated by using Newton's method to minimize the square error between the measured concentration data and the concentration estimates produced with our simulation tool. This Nonlinear Newton's method approach avoids differentiating the measured data, so is far more accurate than the more obvious approach of substituting the measured concentration data into a diffusion-constant parameterized diffusion equation and solving the linear least squares problem. We have also developed a new approach for solving an inverse optical scattering problem associated with the optical inspection of fabricated structures. The method determines the geometric features of a fabricated structure, from spectroscopic ellipsometry measurements, by combining a parameterized low-order model with an optimization algorithm. We make improvements on the polynomial fittingbased parameterized moment matching technique to extract such model automatically. Since the resulting model is inexpensive to evaluate, the method shows large speedup without losing much accuracy: the examples show more than 1000 times speedup with less than 1% error in the final geometric parameter estimation.

We have also developed an approach which merges a recently developed trajectory piecewise-linear (TPWL) model order reduction technique, providing a cost-efficient representation of the nonlinear system, with projection method based on TBR. As shown, this method outperforms algorithms using solely Krylov subspace reduction, while maintaining a relatively low computational cost.

The efficient DSMC method that we have developed, the octant flux splitting information preserving DSMC, overcomes the low-efficiency issue of the classical DSMC method in the applications of low-speed gas flows. This development has made a significant advancement in the DSMC method and has also made the modeling of MEMS/NEMS devices using the accurate molecular based approaches be feasible. The modeling of the Knudsen pump and the thermal sensing Atomic Force Microscope are two examples that have demonstrated the efficiency of the method. In particular, the velocity fields inside both devices and the pressure difference on the cantilever are of small magnitude. These can not be possibly obtained using the classical DSMC method without a tremendously powerful computer. With the developed method, we were able to obtain these fields by just using regular workstations.

Contributions to Other Disciplines:

The developed Integral approaches for nonlinear problems and model order reduction techniques would be useful for a variety of applications in different disciplines, for example, the acoustic field, nonlinear fracture, bioMEMS, design of functional graded materials, etc.

The developed efficient DSMC method and code would be a valubale modeling technique and tool for the modeling and design of various MEMS/NEMS devices with applicaitons ranging from chemical and biological sensors to high-frequency filters and oscillators in wireless communicaiton systems.

Contributions to Human Resource Development:

Mrs. Jian Ding and Mr Nathan Masters have been granted the doctoral degree from Georgia Institute of Technology.
Mr. Dmitry Vasilyev, Mr. Carlos Coelho and Mr. Jung Hoon Lee have been granted the doctoral degree from Massachusetts Institute of Technology.

Contributions to Resources for Research and Education:

Contributions Beyond Science and Engineering:

Categories for which nothing is reported:

Any Web/Internet Site

Contributions: To Any Resources for Research and Education

Contributions: To Any Beyond Science and Engineering